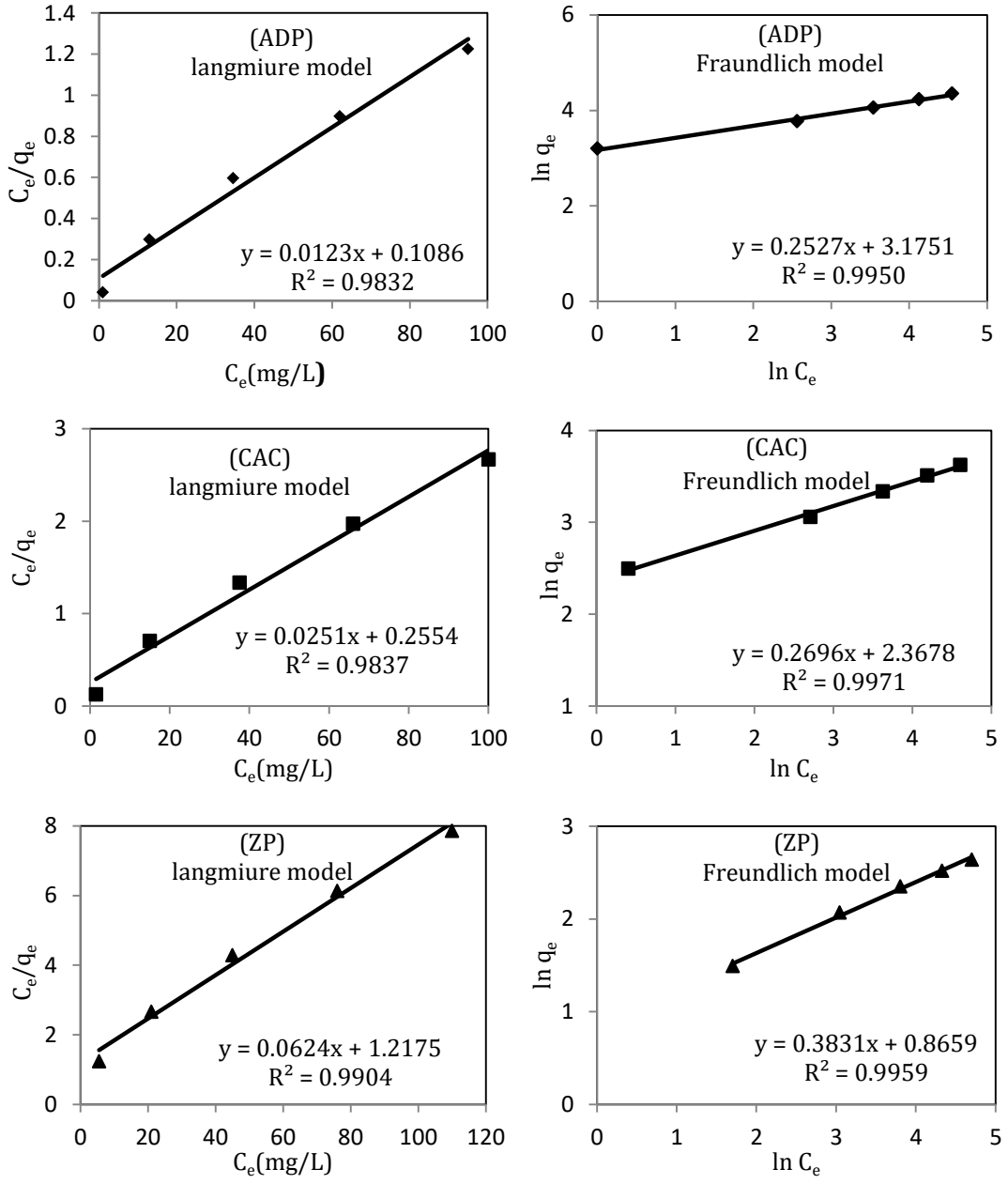


**Fig. S1.** Linear form of isotherm models for sorption of $Pb^{+2}$ onto ADP, CAC, and ZP.

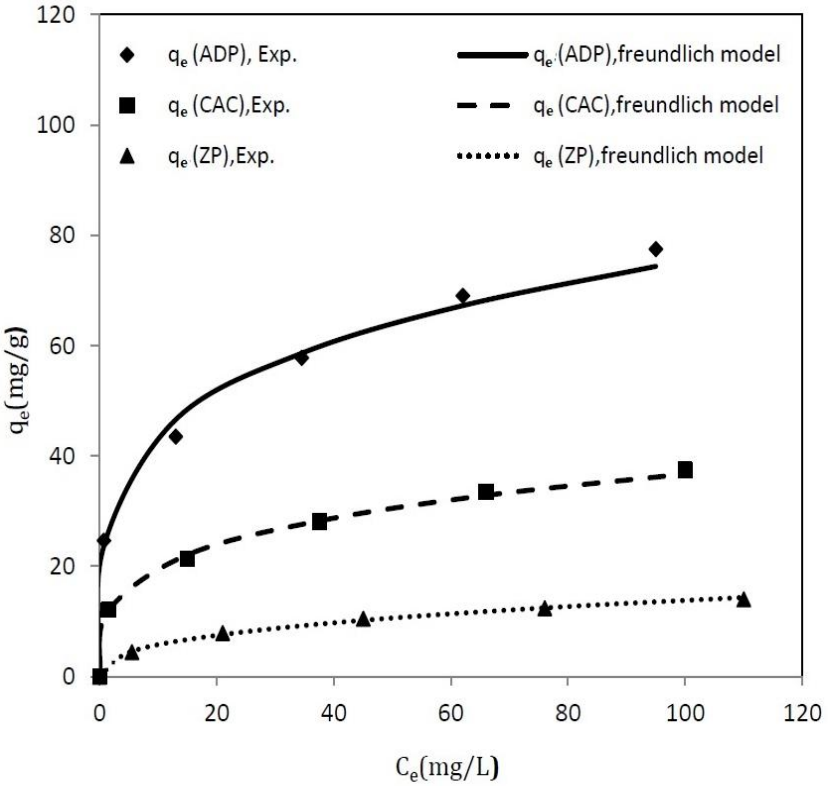


**Fig. S2.** Comparison of the experimental and theoretical result values.

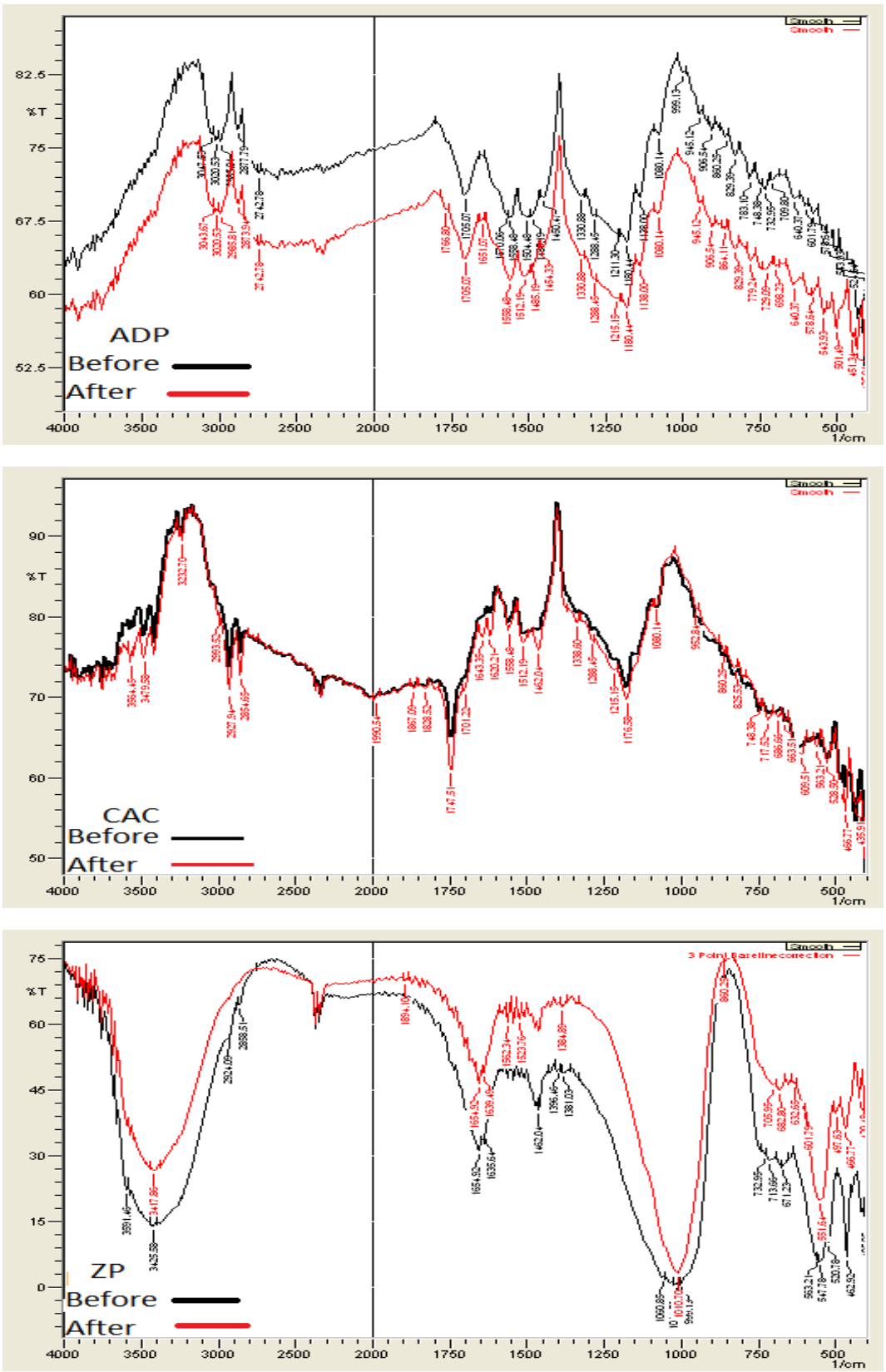


**Fig. S3.** FTIR analysis of ADP, CAC, and ZP before and after sorption of lead.

**Table S1.** Properties of Reactive Materials

| Materials | Physical prosperities | | Chemical prosperities | |
|---|---|---|---|---|
| ADP | Surface area($m^2$/g) | 950 | pH | 6.5 |
| | Bulk density(g/$cm^3$) | 0.251 | Ash content (%) | 4.88 |
| | Porosity | 0.40 | C % | 54.9 |
| | Average particle diameter (mm) | 0.775 | Moisture content % | 7 |
| | pore volume ($cm^3$/g) | 0.921 | Volatile matter (%) | 5 |
| CAC | Surface area($m^2$/g) | 800 | pH | 7.5 |
| | Bulk density(g/$cm^3$) | 0.147 | Ash content (%) | < 5 |
| | Porosity | 0.41 | C % | 68.6 |
| | Average particle diameter (mm) | 0.775 | Moisture content % | 7.8 |
| | pore volume ($cm^3$/g) | 0.76 | Volatile matter (%) | 1.7 |
| ZP | Surface area($m^2$/g) | 520 | pH | 7.5 |
| | Bulk density(g/$cm^3$) | 0.58 | $SiO_2$ | 34.48 |
| | Porosity | 0.39 | $Al_2O_3$ | 29.93 |
| | Average particle diameter (mm) | 0.775 | CaO | 2.54 |
| | Cation exchange capacity (meq/100g) | 1.7 | $Na_2O$ | 0.51 |

**Table S2.** Parameters of Isotherm Models for the Sorption of $Pb^{+2}$ onto ADP, CAC, and ZP.

| Isotherm model | Parameter | ADP | CAC | ZP |
|---|---|---|---|---|
| Langmuir | b (L/mg) | 0.111 | 0.1 | 0.0514 |
| | $q_m$ (mg/g) | 83.33 | 40 | 16 |
| | $R^2$ | 0.9832 | 0.9837 | 0.9904 |
| Freundlich | $K_F$ (mg/g)$(L/mg)^{1/n}$ | 23.93 | 10.66 | 2.375 |
| | n | 3.968 | 3.72 | 2.61 |
| | $R^2$ | 0.9950 | 0.9971 | 0.9959 |

**Table S3.** Functional Groups Responsible for $Pb^{+2}$ Sorption onto ADP, CAC, and ZP

| Materials | Wave NO. ($cm^{-1}$) | Type of bond | Functional group |
|---|---|---|---|
| ADP | 524.64 | $C\text{-}I^-$ | Alkyl halides |
| | 748.38 | $C\text{-}Cl^-$ | Alkyl halides |
| | 1211.3 | $C\text{-}O\text{-}C^-$ | Alcohols |
| | 1450.47 | $-OH^-$ | Carboxylic acid |
| | 2877.79 | $-OH^-$ | Carboxylic acid |
| | 3047.53 | $-OH^-$ | Carboxylic acid |
| CAC | 524.64 | $C\text{-}I^-$ | Alkyl halides |
| | 605.65 | $C\text{-}Cl^-$ | Alkyl halides |
| | 1219.01 | $C\text{-}O\text{-}C^-$ | Alcohols |
| | 1465.9 | $-OH^-$ | Carboxylic acid |
| | 1743.65 | $C=O^-$ | Carboxylic acid |
| | 3251.98 | $-OH^-$ | Carboxylic acid, |
| ZP | 547.78 | Si-O-Si, stretch<br>O-Si-O, bend | $SiO_4$ group |
| | 713.66 | Sym. stretch | $SiO_4$, $AlO_4$ group |
| | 1635.64 | $OH^-$, bend | Hydroxyl group |
| | 3425.58 | $OH^-$, stretch | Hydroxyl group |

**Table S4.** Parameters, Constants, Boundary and Initial Conditions Used in the Transport Modeling of Lead in 2D Model Setup

| Item | Location | Type/Value | |
|---|---|---|---|
| Subdomain settings | Aquifer | Aquifer bed length before barrier = 40 m | |
| | | Aquifer bed length after barrier = 27 m | |
| | | Porosity ($n_A$) = 0.42 | |
| | | X-velocity ($V_A$) = 0.00008 m/s | |
| | | Bulk density ($\rho_b$) = 1.563 g/cm$^3$ | |
| | PRB | Barrier bed thickness = 3m | |
| | | Porosity ($n_B$) = 0.40, 0.41, 0.39 for ADP, CAC, and ZP, respectively | |
| | | X-velocity ($V_B$) = 0,000084, 0.000081, 0.000086 m/s for ADP, CAC, and ZP, respectively * | |
| | | Bulk density ($\rho_b$) = 0.251, 0.147, 0.58 g/cm$^3$ for ADP, CAC, and ZP, respectively | |
| Boundary settings | Upper boundary | No flux/symmetry | |
| | Lower boundary | No flux/symmetry | |
| | Left side boundary | Line source | $C_o$ = 0.05kg/m$^3$ |
| | | Except for the line source | No flux/symmetry |
| | Right side boundary | Advective flux | |
| Initial condition | (X, Y) | Initial concentration = 0 | |

*The velocity in the PRB ($V_B$) is evaluated by the following equation: [$V_A\, n_A = V_B\, n_B$]